ANALYTICAL MODEL FOR INTERGRAIN EXPANSION AND CLEAVAGE: RANDOM GRAIN BOUNDARIES

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A description of rigid-body grain boundary relaxation and cleavage in tungsten is performed using a pair-wise Morse interatomic potential in real and reciprocal spaces. Cleavage energies and grain boundary dilatation of random grain boundaries were formulated and computed using atomic layer interaction energies. These values were determined using a model for a relaxed random grain boundary that consists of rigid grains on either side of the boundary plane that are allowed to float to reach the equilibrium position. Expressions are given that describe in real space the energy of interatomic interaction on random grain boundaries with twist orientation. It was shown that grain-boundary expansion and cleavage energies of the most widespread random grain boundaries are mainly determined by grain boundary atomic density.

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INTRODUCTION

Much insight into the atomic structure of grain boundaries (GBs) has been gained in recent decades using high-resolution methods of electron and field-ion microscopy and computer simulation. Since computer simulations of interfaces usually employ periodic boundary conditions, it is very difficult to study random (general) boundaries. These most widespread interfaces were approximated by near coincidence site lattice (CSL) boundaries with long periods and a high reciprocal density of coincident sites Σ (Σ→∞) [1]. The most of computer simulations of grain-boundary expansion and cleavage have been confined to CSL boundaries with a high degree of regularity and relatively low Σ. GB cleavage is a common failure mechanism in polycrystalline materials, particularly in the presence of embrittling elements (e.g., helium) [1, 2].

A substantial shortcoming of both experimental microscopic techniques and mathematical modeling is that although they make available exceptionally detailed information about the particular GBs under examination, it is usually difficult to deduce systematic trends in structure from one intergrain boundary to another. The simplicity of the pair-wise interatomic potentials is such that it allows an analytic description of the atomic structure and energetics of GBs to be created. As was shown in [3-5], the calculation of the GB energetics performed in reciprocal space make it possible to analytically describe the dependence of the GB energy on atomic structure in the whole space of GB macroscopic degrees of freedom. The GB atomic configurations can be determined in reciprocal space on the basis of a Fourier transform of pair-wise potentials. The first investigation of GB structure using analytical model was performed for pair-wise Lennard-Jones potentials [1, 3]. This study was restricted to analyzing structure-insensitive types of GBs, due to the divergence of the Fourier transform of Lennard-Jones potentials at small distances between atomic planes. In this paper, it is shown that the atomic structure and energetics of the most widespread interfaces in polycrystals – the GB of random (general) type can be described in terms of an analytic model in the real space.

RESULTS AND DISCUSSION

Mathematical simulations were performed using molecular statics with Morse long-range interatomic potential. In the absence of impurities, GBs are generally sharp interface, with the change in crystal orientation taking place within a few atomic layers. So the thickness of the grain boundary simulation box was taken as 30–50 crystallographic planes, parallel to the interface. This thickness was more than an order of magnitude larger than the range of the Morse potential and the GB structural length. Due to the homogeneous tensile strain in the direction, normal to the GB plane and the symmetry of the present cell, all the shear stress components were negligible and can be regarded as zero.

The study in reciprocal space of the interaction atomic layers includes determination of the Fourier transform of the interatomic potential by the integrating extended over two-dimensional net [1, 4]. An analytical expression for the GB energy can be obtained using the effective potential in form

$$v(r) = D\left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}\right], \qquad (1)$$

where D = 0.9906 eV, α = 1.4116 Å^{-1} and r_0= 3.032 Å.

To calculate the total energy of the pair-wise atomic interaction W, a lattice summation must be performed. We use the orthogonal coordinate systems x-y within a plane parallel to the GB. The lattice periods in the x and y directions are a_x, a_y and $\left|\vec{G}\right| = \sqrt{g_{xl}^2 + g_{ym}^2}$ where $g_{xl} = \frac{2\pi l}{a_x}$, $g_{ym} = \frac{2\pi m}{a_y}$ and l, m are summation indices locating points in the planar reciprocal lattice. Here a – is the parameter of three-dimensional lattice. The module of the relative translation may be expressed as $\left|\ \vec{T}_{jk}\ \right| = \sqrt{T_{xjk}^2 + T_{yjk}^2}$,

$$W = 2\pi a\sigma^2 D' \sum_{lm}\sum_{j}\sum_{k} \left\{ \frac{D'}{D}\frac{1}{p_{lm}^3}\left[1 + p_{lm}(z_n - z)\right]e^{-p_{lm}(z_n - z)} - \frac{1}{q_{lm}^3}\left[1 + q_{lm}(z_n - z)\right]e^{-q_{lm}(z_n - z)} \right\} \times \cos(g_x T_{xjk})\cos(g_y T_{yjk}), \quad (2)$$

where $p_{lm} = \sqrt{a^2 + g_x^2 + g_y^2}$, $q_{lm} = \sqrt{b^2 + g_x^2 + g_y^2}$ and $\sigma = (a_x a_y)^{-1}$ is the planar atomic density, z_{jk} is the separation between the 2D-lattices. The position of the atomic layers have been labelled from -25 < *j, k* < 25. The wave-vector numbers were in interval $|l,m| \le 20$. For a close-packed planes, only those terms referring to near-surface planes and having both $|l| \le 4$ and $|m| \le 4$ contribute significantly to the sum in *W*. So the convergence of the series for these planes is high and the method of simulation in reciprocal space is computationally efficient. Random (incommensurate) GBs were produced by a rotation of grains about common low-indices directions. The random GB can be obtained by a reducing the summation to the case *l = m = 0*.

As was shown in Ref. [6] that the discreteness of the GB energy characteristics was rapidly destroyed with increasing Σ value towards an asymptotic form, referred to as the random-boundary limit. In this case interacting atoms are assumed to be randomly distributed within the crystallographic planes of the adjacent grains separated by the distance *z* (Fig. 1).

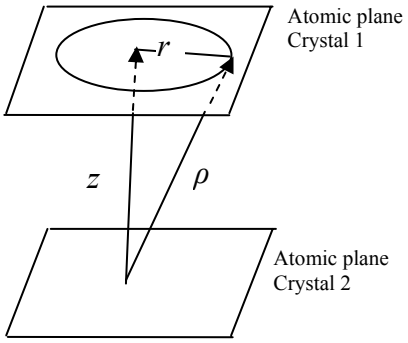

Fig. 1. Scheme of interatomic interaction in the random-boundary limit

According to Fig. 1, the number of atoms in crystal 1 interacting with an atom of crystal 2 in the interval *r, r+dr* is equal to $2\pi\sigma r dr$, where $r^2+z^2=\rho^2$, *z* is the distance between atomic planes. Assuming the interatomic interaction is of the Morse type (Eq. (1)), the energy of interaction of an atom crystal 2 with all atoms in crystal 1 can be written in the form

$$w_a = D\sigma \int_0^{2\pi}\int_0^{\infty} \left[e^{-2\alpha(\rho - r_0)} - 2e^{-\alpha(\rho - r_0)}\right] \cdot r dr d\varphi = 2\pi D\sigma \int_0^{\infty} r\left[e^{2\alpha\cdot r_0}e^{-2\alpha\cdot\rho} - 2e^{\alpha\cdot r_0}e^{-\alpha\cdot\rho}\right]dr. \quad (3)$$

Performing the change of the variable of integration according to Fig. 1, we obtain

$$w_a = 2\pi D\sigma \int_z^{\infty} \rho\left[e^{2\alpha\cdot r_0}e^{-2\alpha\cdot\rho} - 2e^{\alpha\cdot r_0}e^{-\alpha\cdot\rho}\right]d\rho = 2\pi D\sigma\left[\frac{1}{4}e^{2\alpha\cdot r_0}\int_{2z}^{\infty}\rho\cdot e^{-\alpha\cdot\rho}d\rho - 2e^{\alpha\cdot r_0}\int_z^{\infty}\rho\cdot e^{-\alpha\cdot\rho}d\rho\right]. \quad (4)$$

The expression (4) gives the energy of interaction of an atom in plane 1 with all atoms in plane 2. The energy of interaction of all atoms in both planes is obviously equal to:

$$W_p = w_a\sigma. \quad (5)$$

By taking integral (4), in view of Eq. (5) we obtain

$$W_p = 2\pi D\sigma^2\left[\frac{1}{4}\left(\frac{1}{\alpha^2} + \frac{2z}{\alpha}\right)\cdot e^{-2\alpha(z - r_0)} - 2\left(\frac{1}{\alpha^2} + \frac{z}{\alpha}\right)\cdot e^{-\alpha(z - r_0)}\right]. \quad (6)$$

Fig. 2 shows the dependence of the interaction energy of atoms in two crystallographic planes (100) of grains with the twist random GB, calculated by using the reciprocal space Eq. (2) and real space calculations using the real space Eq. (6) on GB dilatation *l*.

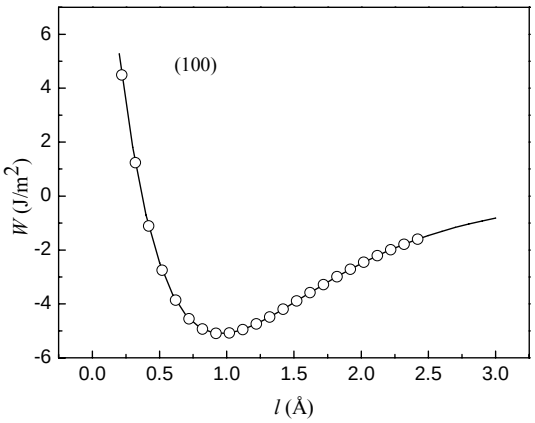

Fig. 2. Dependence of the interaction energy of atoms in two planes (100) of grains with the random GB, calculated by using the reciprocal space equation (2) (curve) and real space calculations using the real space equation (6) (shown by circles) on dilatation

At last, the full interaction energy W in all crystallographic planes (100) of grains with the twist random GB, calculated by using the real space calculations using the real space equation (6) can be written in the form:

$$W = 2\pi D\sigma^2 \sum_{j,k} \left[\begin{array}{l} \frac{1}{4}\left(\frac{1}{\alpha^2} + \frac{2z_{j,k}}{\alpha}\right) \cdot e^{-2\alpha(z_{j,k}-r_0)} - \\ 2\left(\frac{1}{\alpha^2} + \frac{z_{j,k}}{\alpha}\right) \cdot e^{-\alpha(z_{j,k}-r_0)} \end{array} \right], \qquad (7)$$

where $z_{j,k}$ is the distance between j и k plains of both grains.

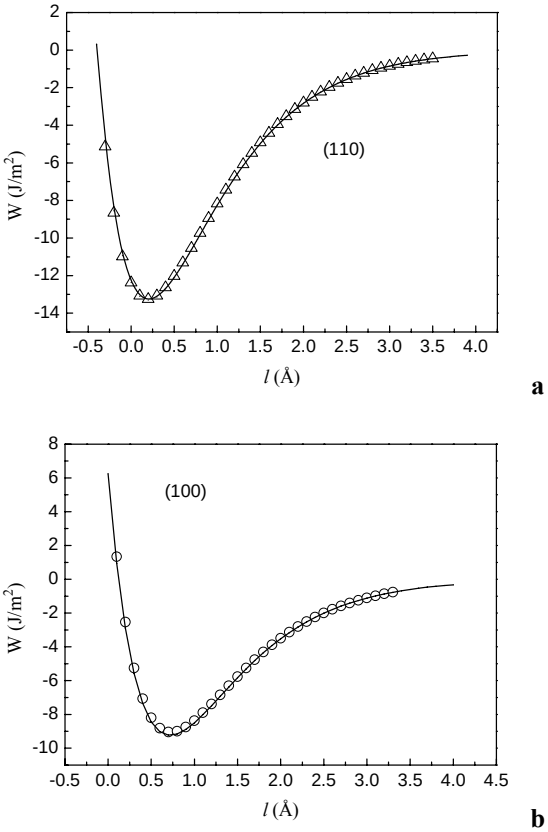

Fig. 3. Dependence of the interaction energy of atoms in all crystallographic planes of both grains with the twist random GB, calculated for the (110) (a) and (100) (b) GB by using the reciprocal space equation and the real space equation (7)

The values shown in Figs. 3–5 were calculated using a model for a relaxed random grain boundary that consists of rigid grains on either side of the boundary plane that are allowed to float to reach the equilibrium position. Both methods in real and reciprocal spaces give the same values of the adhesion energy (or cleavage energy): 13.25 J/m^2 for the (110) random GB and 9.04 J/m^2 for the (100) random GB. In both cases the minimum energy corresponds to the grain boundary dilatation of 0.19 Å for the (110) random GB and 0.68 Å for the (100) random GB. The grain-boundary expansion and cleavage energies of the most widespread random grain boundaries are mainly determined by grain boundary atomic density σ according to Eq. (7).

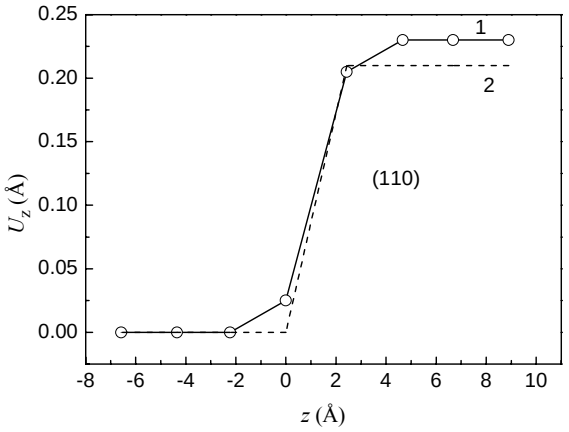

Fig. 4. Grain boundary dilatation calculated for atomic planes with different x-coordinates, calculated for fully relaxed configuration in reciprocal space (1) and for rigid relaxation calculated in real space (2) for the (110) random GB

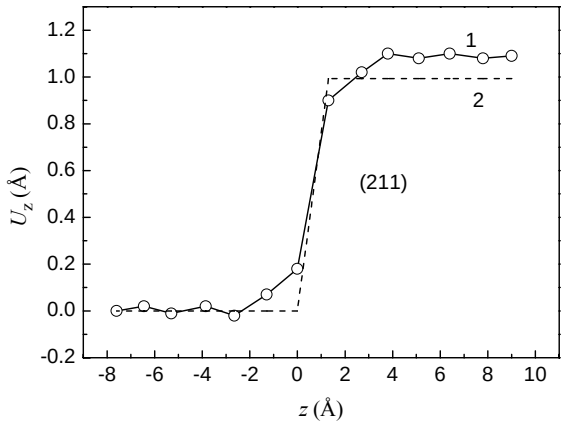

Fig. 5. Grain boundary dilatation calculated for atomic planes with different x-coordinates, calculated for fully relaxed configuration in reciprocal space (1) and for rigid relaxation calculated in real space (2) for the (211) random GB

CONCLUSIONS

Expressions are given that describe in real space the energy of interatomic interaction on random grain boundaries with twist orientation. Cleavage energies and grain boundary dilatation of random grain boundaries were particularly easy to formulate and compute using atomic layer interaction energies in real space. By comparison with full atomic relaxations calculated in reciprocal space for random grain boundaries we have shown that derived expressions that describe in real space the energy of interatomic interaction on random grain boundaries with twist orientation give an adequate description of the grain boundary dilatation. It was shown that the grain-boundary expansion and cleavage energies of the most widespread random grain boundaries are mainly determined by grain boundary atomic density.

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АНАЛИТИЧЕСКАЯ МОДЕЛЬ МЕЖЗЕРЕННОЙ ДИЛАТАЦИИ И РАЗРУШЕНИЯ: ГРАНИЦЫ ЗЕРЕН ПРОИЗВОЛЬНОГО ТИПА

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С использованием парного межатомного потенциала Морза при расчетах в реальном и обратном пространствах получено описание жесткой зернограничной релаксации и разрушения в вольфраме. Сформулирована модель взаимодействия атомных слоев на границах зерен, на основании которой рассчитаны энергии разрушения и межзеренная дилатация границ зерен произвольного типа. Данные величины получены с использованием модели релаксации произвольных границ, допускающей жесткие смещения зерен по обе стороны от границы с целью достижения равновесного положения. Приведены выражения для энергии межатомного взаимодействия в реальном пространстве на границах зерен произвольного типа, описываемых разориентацией кручения. Показано, что межзеренная дилатация и энергия разрушения границ произвольного типа определяются атомной плотностью на границах зерен.

АНАЛІТИЧНА МОДЕЛЬ МІЖЗЕРЕННОЇ ДИЛАТАЦІЇ ТА РУЙНУВАННЯ: МЕЖИ ЗЕРЕН ДОВІЛЬНОГО ТИПУ

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З використанням парного міжатомного потенціалу Морза при розрахунках у реальному і зворотному просторах отримано опис жорсткої зерномежевої релаксації і руйнування у вольфрамі. Сформульовано модель взаємодії атомних шарів на межах зерен, на підставі якої розраховані енергії руйнування і міжзеренна дилатація меж зерен довільного типу. Дані величини отримані з використанням моделі релаксації довільних меж, що допускає жорсткі зміщення зерен по обидві сторони від межі з метою досягнення рівноважного положення. Наведено вирази для енергії міжатомної взаємодії в реальному просторі на межах зерен довільного типу, описуваних розорієнтацією кручення. Показано, що міжзеренна дилатація і енергія руйнування меж довільного типу визначаються атомною густиною на межах зерен.